One-particle exchange in the double folded potential in a semiclassical approximation

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Abstract

The one-particle exchange in the double folded model is analyzed. To this aim the Extended Thomas-Fermi approach to the one-body density matrix is used. The nucleon-nucleon force with Yukawa, Gauss and Coulomb-type form factors are considered. The energy dependence of the exchange part of the double folded potential is investigated and a comparison of the present approach with former ones is carried out.

1 Introduction

Up to the present moment the Double Folded Model (DFM) [1, 3, 4], which starts from the effective nucleon-nucleon force and the single particle densities of the colliding nuclei, has become one of the most popular methods to calculate the real part of microscopic the Heavy-Ion (HI) optical potential. It is also known that folding methods are widely used in other problems of HI Physics [2]. While in the original DFM the antisymmetrization effects were taken into account by means of the effective zero-range pseudopotential , in the latest versions of the DFM the antisymmetrization has been explicitly considered [1, 3, 4]. It is assumed that the structure of of each isolated nucleus is described at Hartree-Fock (HF) level and that the exchange effects come from the non-diagonal part of the single-particle density matrix (DM). The intrinsic states of isolated nuclei are modified during the interaction. However in the DFM the so called "frozen density approximation", which implies that the intrinsic states of the nuclei do not change during the interaction, is assumed.

Thus the key point in the DFM is to express the non-diagonal part of the DM through its diagonal part or, in other words, in a Local Density Approximation (LDA) for DM. The simplest LDA is the Slater (SL) approach to the DM, which is equivalent to the Thomas-Fermi approach, valid in nuclear matter, and does not take into account the nuclear surface effects. A more elaborated LDA is given by the Density Matrix Expansion (DME) of Negele and Vautherin (NV) [5]. Another approach widely used in DFM [4, 6] is the Campi-Bouassy (CB) [7] approximation, in which by a proper choice of the effective momenta in the DME of NV, reduces to the SL form.

The physical quantities that enter into the NV and CB approaches are just the Fermi momentum k_F and the kinetic energy density τ. In the HF method the single-particle density ρ as well as k_F and τ are determined selfconsistently. However, the attractive feature of DFM is to consider ρ as an input data. While the densities ρ can be obtained from the electron scattering data, k_F and τ should be defined theoretically. At present, the values of k_F and τ that correspond to a given single-particle density ρ are unknown. To determine them via ρ, approximate schemes are in order. In particular the Extended Thomas-Fermi (ETF) approach is widely used to this end:

$$k_F = \left(\frac{3\pi^2\rho}{2}\right)^{1/3} \tag{1}$$

and

$$\tau = \frac{3}{5}(\frac{3\pi^2}{2})^{2/3}\rho^{5/3} + \frac{1}{36}\frac{(\nabla\rho)^2}{\rho} + \frac{1}{3}\Delta\rho \tag{2}$$

if a degeneracy 4 is assumed.

Very recently the ETF approximation has been used for deriving the semiclassical one-body density matrix up to $\hbar^2$ order in the case of a non-local single-particle potential [8]. This ETF DM is obtained starting from the Wigner-Kirkwood distribution function for a non-local one-body Hamiltonian [9]. As is shown in [8], the NV and CB approaches to the DM with τ calculated in the ETF approach, are just truncations of the full ETF DM. Consequently, it seems appealing to use the complete semiclassical DM to obtain the real part of the ion-ion potential and compare these results with former potentials obtained using these semiclassical NV and CB approximations.

In the present paper we apply the ETF DM [8] for calculating the DFM potential. We obtain analytical expressions for the potential using the Gogny [10], M3Y [1] and Coulomb forces. To check the validity of our ETF approximation, we analyze the ^{16}O- ^{16}O reaction. The ground state of each isolated ^{16}O nucleus is described using harmonic oscillator (HO) wavefunctions. In this case the quantal DFM potential can be calculated explicitly [11] and we compare this quantal potential with the semiclassical DFM potential obtained using the ETF, SL and CB approximations to the DM.

The paper is organized as follows. In the first section we present the analytical derivation of the semiclassical DFM potential using the SL, CB and ETF approximations to the DM and Gauss, Yukawa and Coulomb form factors for the nucleon-nucleon force. In the next section we compare these semiclassical DFM nucleus-nucleus potentials obtained using several prescriptions for the density of eachisolated nucleus with the corresponding quantal potential. This comparison is done for the ^{16}O-^{16}O reactions. The summary and conclusions are given in the last section.

2 Formalism

In order to obtain the HI potential in the DFM, one can start from its microscopic definition

$$V(D) = \sum_{i\in 1, j\in 2} [< ij|v|ij > - < ij|v|ji >], \tag{3}$$

where i and j represent single particle states of the first- and second-nuclei respectively and v is the effective nucleon-nucleon force. Formally (3) coincides with the corresponding term in the HF method. However in the DFM approach, the single-particle wave functions $|i >$ and $|j >$ are determined selfconsistently only inside each nucleus independently. To take into account the relative motion in the plane wave approximation one should multiply $|i >$ by a factor $exp(i\boldsymbol{k}_1\boldsymbol{r_i})$ in the first nucleus and $|j >$ by $exp(i\boldsymbol{k}_2\boldsymbol{r}_j)$ in the second. Here $\boldsymbol{k}_1 = \boldsymbol{K}_1/A_1$, $\boldsymbol{k}_2 = \boldsymbol{K}_2/A_2$ and $\boldsymbol{K}_\alpha(\alpha = 1, 2)$ is the centre-of-mass moment of the first and second nucleus respectively. The relative momentum between a pair of nucleons of different nuclei is given by : $\boldsymbol{K} = \boldsymbol{k}_1 - \boldsymbol{k}_2$. Its modulus can be defined globally as $K^2 = 2m\mu E_{cm}/\hbar^2$ or locally as [3]: $K^2 = 2m\mu(E - V - V_{Coul})/\hbar^2$, where $\mu = A_1A_2/(A_1 + A_2)$. In the local definition the set of equations: $V = V(K); K = K(V)$ should be solved selfconsistently.

The direct part of the HI potential is given by the first matrix element of (3) and reads:

$$V_{dir}(D) = X_d \int d\vec{r}_1 d\vec{r}_2 \rho_1(\vec{r}_1)\rho_2(\vec{r}_2 - \vec{D})v(s), \tag{4}$$

where $\boldsymbol{s} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The direct part of the HI potential eq.(4) is just the convolution of the single-particle densities ρ_i with the form factor $v(s)$ of the central effective nucleon-nucleon force v. The constant X_d is just the standard combination of the exchange parameters of the central nucleon-nucleon force: $X_d = w + b/2 - h/2 - m/4$. This contribution is easily calculated numerically. It is important to note that the direct part of the HI potential 4 does not depend on energy if the nucleon-nucleon interaction v is energy independent.

The finite-range exchange part of the HI potential is given by:

$$V_{ex}(D, K) = X_e \int d\vec{r}_1 d\vec{r}_2 \rho_1(\vec{r}_1, \vec{r}_2)\rho_2(\vec{r}_2 - \vec{D}, \vec{r}_1 - \vec{D})v(s)e^{i\boldsymbol{K}\boldsymbol{s}}. \tag{5}$$

Here, as usual, $X_e = m + h/2 - b/2 - w/4$. To obtain this term a LDA for the density matrix is used. The simplest LDA is the SL approach, which in terms of centre-of-mass $\boldsymbol{R} = (\boldsymbol{r_1} + \boldsymbol{r_2})/2$ and relative $\boldsymbol{s}$ coordinates reads as:

$$\rho(\vec{r}_1, \vec{r}_2) = \rho(\boldsymbol{R})\frac{3j_1(k_F s)}{k_F s}, \tag{6}$$

where the Fermi momentum k_F is related to the density by the usual Thomas-Fermi relation (1) (Here we use degeneracy factor 4 so the single particle density ρ is normalized to the mass number). This approximation is exact at HF level in infinite nuclear matter. To take into account finite size effects of the nuclei some modifications have to be made. Among different approaches to the DM, in the present paper we consider the Campi-Bouyssy (CB) [7] one that is often used in DFM calculations. In the CB approximation the DM has the same form as the SL term (3), but instead of the Fermi momentum k_F, uses an effective momentum $\tilde{k}$ defined as:

$$\tilde{k}^2 = \frac{5}{3\rho(\boldsymbol{R})}(\tau(\boldsymbol{R}) - \frac{1}{4}\Delta\rho(\boldsymbol{R})). \tag{7}$$

In this equation τ is just the exact quantal kinetic energy density. Consequently, to calculate it one needs to know the exact DM. To overcome this difficulty some approximate schemes for τ are used, often they are based on its ETF value eq.(2) [11].

Let us now derive the exchange term (5) using the ETF approach to the DM [8] for each isolated nucleus. This DM averaged over $\boldsymbol{s}$ can be written as:

$$\rho(\vec{R}, s) = \rho_{TF}(\boldsymbol{R}, s) + \delta\rho(\boldsymbol{R}, s), \tag{8}$$

where ρ_{TF} is the Thomas-Fermi term, which is equivalent to the SL approximation (6). The averaged second-order semiclassical correction $\delta\rho$ that we will use in this work reads as:

$$\delta\rho = \frac{s^2}{72}\{\Delta\rho[j_0(k_F s) - \frac{6j_1(k_F s)}{k_F s}] - \frac{(\nabla\rho)^2}{\rho}[\frac{4}{3}j_0(k_F s) - 3\frac{j_1(k_F s)}{k_F s}]\}. \tag{9}$$

In this approximation all the quantities are defined in a unique way. Eq.(9) gives the ETF-$\hbar^2$ correction to the DM in the case of a local HF potential. To take into account the non-locality of the single particle mean field, one should consider effective masscorrections in $\delta\rho$. This case is analyzed in [8] in detail. It is also shown that the contribution of these non-local effects to the $\hbar^2$ part of the DM are rather small as compared with the full $\hbar^2$ correction if realistic finite-range forces are used. Therefore we will not consider the effective mass corrections to $\delta\rho$ in this paper. We calculate the DFM potential using nucleon-nucleonforces with a Gauss, Yukawa and Coulomb-type form factors which cover most of the effective interactions used in DFM calculations. As typical examples we will consider the Gogny [10] and M3Y forces [1].

2.1 Gaussian-type force

Let us consider a central nucleon-nucleon force with a Gaussian form factor:

$$v(s) = v_0 exp(-\frac{s^2}{\mu^2}). \tag{10}$$

The exchange contribution to the DFM potential is given by:

$$V_{ex}(D) = X_e v_0 \int d^3r \{\tilde{V}_{Sl}(k[r]) + \delta\tilde{V}(k[r])\}, \tag{11}$$

where the SL term $\tilde{V}_{Sl}$ is given by

$$\begin{aligned}
\tilde{V}_{Sl} &= -\frac{9\pi^2\rho_1\rho_2}{2Kk_1^3k_2^3}\sum_\alpha\{[-\sigma_1\sigma_2(\frac{\alpha^4}{24}+\frac{\alpha^2}{2\mu^2}+\frac{1}{2\mu^4}) \\
&+(\sigma_2k_1+\sigma_1k_2)(\frac{\alpha^3}{6}+\frac{\alpha}{\mu^2})-k_1k_2(\frac{\alpha^2}{2}+\frac{1}{\mu^2})]erf(\frac{\mu}{2}\alpha) \\
&+[-\sigma_1\sigma_2(\frac{\alpha^3}{12\mu^2}+\frac{5\alpha}{6\mu^4})+(\sigma_2k_1+\sigma_1k_2)(\frac{\alpha^2}{3\mu^2}+\frac{4}{3\mu^4}) \\
&-k_1k_2\frac{\alpha}{\mu^2}]\frac{\mu}{\sqrt{\pi}}exp[-\frac{\mu^2}{4}\alpha^2]\}.
\end{aligned} \tag{12}$$

Here $\sigma_{1,2}$ is the sign of $k_{1,2}$ (which are the Fermi momentum k_F of each nucleus related to the corresponding density through eq.(1)), while $\alpha = K \pm k_1 \pm k_2$. The summation in (12) is taken over all possible α. The explicit form of (12) is given in [12]. To calculate the DFM potential in the CB approach we use the effective momentum (7) with the semiclassical ETF kinetic energy density (2).

The second-order correction to the DFM is given by:

$$\begin{aligned}
\delta\tilde{V}(R) &= -\frac{1}{36\pi^2K}\{(-k_1f_1-k_2f_2)\sum_\alpha\sigma_1\sigma_2erf(\frac{\mu}{2}\alpha) \\
&+\frac{\mu k_1k_2}{\sqrt{\pi}}[(f_1+f_2)(exp[-\frac{\mu^2(K+x_1)^2}{4}]-exp[-\frac{\mu^2(K-x_1)^2}{4}]) \\
&+(f_1-f_2)(exp[-\frac{\mu^2(K+x_2)^2}{4}]-exp[-\frac{\mu^2(K-x_2)^2}{4}])] \\
&-3(\frac{g_1}{k_1}+\frac{g_2}{k_2})[[\frac{1}{2}(K^2-k_1^2-k_2^2)+\frac{1}{\mu^2}]\sum_\alpha(\sigma_1)(\sigma_2)erf[\frac{\mu\alpha}{2}] \\
&+\frac{1}{\sqrt{\pi}\mu}\sum_\alpha\sigma_1\sigma_2\alpha^- exp[-\frac{\mu^2}{4}\alpha^2]]\},
\end{aligned} \tag{13}$$

where $\alpha^- = K \mp k_1 \mp k_2$, $x_1 = k_1 + k_2$, $x_2 = k_1 - k_2$ and

$$f_i = \Delta k_i - 2\frac{(\nabla k_i)^2}{k_i} = \frac{\pi^2}{2k_i^2}[\Delta\rho_i - \frac{4}{3}\frac{(\nabla\rho_i)^2}{\rho_i}] \tag{14}$$

$$g_i \;=\; 2\Delta k_i + \frac{(\nabla k_i)^2}{k_i} = \frac{\pi^2}{2k_i^2}[2\Delta\rho_i - \frac{(\nabla\rho_i)^2}{\rho_i}].$$

Let us now analyze these formulas. We will talk about the high energy limit when $K/k_i >> 1, i = 1, 2$ which is valid at high enough energy. However, it could also be valid at small energies in the outer region of nuclei when they overlap weakly. One can see that in this regime the SL term dominates and the h^2 correction is negligible.

$$\tilde{V}_{Sl} = -\frac{3\pi^{3/2}\rho_1\rho_2}{8k_1^3k_2^3}\mu^3K^4k_1k_2e^{-\frac{\mu^2K^2}{4}} + O([\frac{k_i}{K}]^2]). \tag{15}$$

On the contrary, at small energies the h^2 correction plays an important role. The SL term in the low energy limit, e.g. when $\frac{K}{k_i} << 1$, looks like

$$\begin{aligned}\tilde{V}_{Sl} \;=\; & -\frac{9\pi^2\rho_1\rho_2}{2k_1^3k_2^3}\{\frac{2}{3}(k_1^3+k_2^3)erf[\frac{\mu}{2}(k_1+k_2)] - \frac{2}{3}(k_1^3-k_2^3)erf[\frac{\mu}{2}(k_1-k_2)] \\ & +\frac{1}{\mu\pi}[\frac{8}{3\mu^2}(exp[-\frac{\mu^2}{4}(k_1-k_2)^2] - exp[-\frac{\mu^2}{4}(k_1+k_2)^2]) \\ & +\frac{4}{3}(k_1+k_2)^2exp[(-\frac{\mu^2}{4}(k_1+k_2)^2] - \frac{4}{3}(k_1-k_2)^2exp[(-\frac{\mu^2}{4}(k_1-k_2)^2] \\ & -4k_1k_2(exp[-\frac{\mu^2}{4}(k_1-k_2)^2] + exp[-\frac{\mu^2}{4}(k_1+k_2)^2])]\} + O([\frac{K}{k_i}]^2).\end{aligned} \tag{16}$$

This formula was obtained in [13] for the static SL DFM potential with the Gogny force. The low energy limit of the $\hbar^2$ correction is:

$$\begin{aligned}\delta\tilde{V}(R) \;=\; & -\frac{\mu}{36\pi^{5/2}}\{[3(\frac{g_1}{k_1}+\frac{g_2}{k_2})[(k_1^2+k_2^2) - \frac{4}{\mu^2}] - 2(k_1f_1+k_2f_2)] \\ & \times[exp[-\frac{\mu^2}{4}(k_1+k_2)^2] - exp[-\frac{\mu^2}{4}(k_1-k_2)^2]] \\ & -3(\frac{g_1}{k_1}+\frac{g_2}{k_2})[(k_1+k_2)^2\exp[-\frac{\mu^2}{4}(k_1+k_2)^2] \\ & -(k_1-k_2)^2\exp[-\frac{\mu^2}{4}(k_1-k_2)^2]] \\ & -\mu^2k_1k_2[(k_1+k_2)(f_1+f_2)exp[-\frac{\mu^2}{4}(k_1+k_2)^2] \\ & +(k_1-k_2)(f_1-f_2)exp[-\frac{\mu^2}{4}(k_1-k_2)^2]]\} + O((\frac{K}{k_i})^2).\end{aligned} \tag{17}$$

In a realistic calculation both limiting cases: $K/k_i << 1$ and $k_i/K << 1$ could take place at the same relative energy, but at different points in space.

2.2 Yukawa-type force

For a Yukawa-type force

$$v(s) = v_0 \frac{e^{-\beta s}}{\beta s} \tag{18}$$

one will get

$$\begin{aligned}
\tilde{V}_{Sl} &= -\frac{9\pi\rho_1\rho_2}{K\beta k_1^3 k_2^3}\{\frac{1}{30}K^3 k_1 k_2 + \frac{11}{30}(k_1^2+k_2^2)Kk_1k_2 - \frac{1}{10}\beta^2 K k_1 k_2 \\
&+\sum[-\sigma_1\sigma_2(\frac{\alpha^2\beta^3}{12} - \frac{\alpha^4\beta}{24} - \frac{\beta^5}{120}) \\
&+(\sigma_2 k_1 + \sigma_1 k_2)(\frac{\alpha\beta^3}{6} - \frac{\alpha^3\beta}{6}) + k_1k_2(\frac{\alpha^2\beta}{2} - \frac{\beta^3}{6})]arctg(\frac{\alpha}{\beta}) \\
&+[-\sigma_1\sigma_2(\frac{\alpha^5}{120} + \frac{\alpha\beta^4}{24} - \frac{\alpha^3\beta^2}{12}) \\
&+(\sigma_2 k_1 + \sigma_1 k_2)(\frac{\alpha^4}{24} - \frac{\alpha^2\beta^2}{4} + \frac{\beta^4}{24}) + k_1k_2(\frac{\alpha\beta^2}{2} - \frac{\alpha^3}{6})]J_1^c(\alpha)\},
\end{aligned} \tag{19}$$

where only the combination

$$J_1^c(\alpha_1) - J_1^c(\alpha_2) = \int \frac{ds}{s}[cos(\alpha_1 s) - cos(\alpha_2 s)]exp(-\beta s) = \frac{1}{2}ln\frac{\alpha_2^2+\beta^2}{\alpha_1^2+\beta^2}$$

appears. Again if one uses the CB effective momenta one will get the CB approximation to the DFM. The explicit expression of (19) can be found in [12]. The second-order correction to the DFM potential is:

$$\begin{aligned}
\delta\tilde{V} &= -\frac{1}{18\pi^3\beta K}\{2Kk_1k_2(\frac{g_1}{k_1}+\frac{g_2}{k_2}) \qquad (20)\\
&+[\beta(k_1f_1+k_2f_2) - (\frac{\beta^3}{2} + \frac{3\beta}{2}(k_1^2+k_2^2) - \frac{3\beta}{2}K^2)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]\sum_\alpha \sigma_1\sigma_2 arctg(\frac{\alpha}{\beta}) \\
&+[\frac{K}{2}(k_1f_1+k_2f_2) + (\frac{K^3}{4} - \frac{3K}{4}(k_1^2+k_2^2+\beta^2))(\frac{g_1}{k_1}+\frac{g_2}{k_2}) \\
&\times[ln\frac{(K+x_1)^2+\beta^2}{(K+x_2)^2+\beta^2} + ln\frac{(K-x_1)^2+\beta^2}{(K-x_2)^2+\beta^2}] \\
&+[\frac{1}{2}(k_1^2f_1+k_2^2f_2) - \frac{1}{2}(k_1^3+k_2^3)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(K+x_1)^2+\beta^2}{(K-x_1)^2+\beta^2} \\
&-[\frac{1}{2}(k_1^2f_1-k_2^2f_2) - \frac{1}{2}(k_1^3-k_2^3)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(K+x_2)^2+\beta^2}{(K-x_2)^2+\beta^2}\}. \qquad (21)
\end{aligned}$$

Considering the high energy limit, where the $\hbar^2$ correction to the potential is negligible, one will get

$$\tilde{V}_{Sl} = -\frac{4\pi}{\beta K^2}\rho_1(\vec{r})\rho_2(\vec{r}-\vec{R}) + O([\frac{k_i}{K}]^4). \tag{22}$$

These results for a Yukawa force correspond to the convolution of the densities of the isolated nuclei with a zero-range pseudopotential and an extra $1/E$ energy-dependence. Therefore at high enough energy, when $K/k_i > 1$, a simple zero-range pseudopotential can be used for calculating the exchange part of the DFM potential in this case. The parameters of this pseudopotential are determined by the range β of the effective nucleon-nucleon force (here M3Y). The inverse energy dependence in (22) should be taken into account.

Now we consider the low energy limit where h^2 correction is more important. The SL term in this case looks like:

$$\begin{aligned}
\tilde{V}_{Sl} &= -\frac{9\pi\rho_1\rho_2}{\beta k_1^3 k_2^3}\{k_1k_2[\frac{11}{30}(k_1^2+k_2^2) - \frac{1}{10}\beta^2 \\
&+ \frac{1}{Q}[\frac{16\beta^2}{15}k_1^2k_2^2 + \frac{\beta^2}{3}(k_1^2-k_2^2)^2 - \frac{\beta^6}{15} + \frac{2}{15}(k_1^2-k_2^2)^2(k_1^2+k_2^2-\beta^2)]] \\
&- \frac{2\beta}{3}[(k_1^3+k_2^3)arctg(\frac{k_1+k_2}{\beta}) - (k_1^3-k_2^3)arctg(\frac{k_1-k_2}{\beta})] \\
&+ (\frac{\beta^4}{24} + \frac{\beta^2}{4}(k_1^2+k_2^2) - \frac{1}{8}(k_1^2-k_2^2)^2)\ln\frac{(k_1+k_2)^2+\beta^2}{(k_1-k_2)^2+\beta^2}\} + O((\frac{K}{k_i})^2).
\end{aligned} \tag{23}$$

The corresponding $\hbar^2$ correction reads:

$$\begin{aligned}
\delta\tilde{V} &= -\frac{1}{9\pi^3\beta}\{3k_1k_2(\frac{g_1}{k_1}+\frac{g_2}{k_2}) \\
&- \frac{2k_1k_2}{Q}[\beta^2(k_1f_1+k_2f_2) + (k_1^2-k_2^2)(k_1f_1-k_2f_2)] \\
&+ \frac{1}{2}[(k_1f_1+k_2f_2) - \frac{3}{2}(k_1^2+k_2^2+\beta^2)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(k_1+k_2)^2+\beta^2}{(k_1-k_2)^2+\beta^2}\} + O([\frac{K}{k_i}]^2),
\end{aligned} \tag{24}$$

where

$$Q = \beta^4 + 2\beta^2(k_1^2+k_2^2) + (k_1^2-k_2^2)^2 \tag{25}$$

2.3 Coulomb force

Let us now consider the Coulomb force:

$$v(s) = \frac{e^2}{r} \tag{26}$$

In this particular case one will get the explicit expression for the SL term:

$$\tilde{V}_{Sl} = -\frac{9\pi e^2\rho_1\rho_2}{Kk_1^3k_2^3}\{\frac{1}{30}K^3k_1k_2 + \frac{11}{30}(k_1^2+k_2^2)Kk_1k_2$$

$$+[\frac{K^5}{240}-\frac{K^3}{24}(k_1^2+k_2^2)-\frac{K}{16}(k_1^2-k_2^2)^2][ln\frac{(K+k_1+k_2)^2}{(K+k_1-k_2)^2}+ln\frac{(K-k_1-k_2)^2}{(K-k_1+k_2)^2}]$$
$$-[\frac{K^2}{12}(k_1^3+k_2^3)+\frac{1}{60}(k_1+k_2)^3[(k_1-k_2)^2-k_1k_2]]ln\frac{(K+k_1+k_2)^2}{(K-k_1-k_2)^2}$$
$$+[\frac{K^2}{12}(k_1^3-k_2^3)+\frac{1}{60}(k_1-k_2)^3[(k_1+k_2)^2+k_1k_2]]ln\frac{(K+k_1-k_2)^2}{(K-k_1+k_2)^2}\},\qquad(27)$$

where now ρ_i and k_i (i=1,2) correspond to the density and Fermi momentum of protons in each nucleus: $\rho_i=\rho_{i,p}$, $k_i=k_{i,p}$. On first sight of (25) one can think that at $K=\pm k_1\pm k_2$ this formula contains divergent terms. However, one can see that the corresponding terms that appears twice cancel each other.

The second-order correction to the DFM potential is:

$$\begin{aligned}\delta\tilde{V} &= -\frac{e^2}{18\pi^3K}\{2Kk_1k_2(\frac{g_1}{k_1}+\frac{g_2}{k_2})\\
&+[\frac{K}{2}(k_1f_1+k_2f_2)+(\frac{K^3}{4}-\frac{3K}{4}(k_1^2+k_2^2))(\frac{g_1}{k_1}+\frac{g_2}{k_2})\\
&\times[ln\frac{(K+x_1)^2}{(K+x_2)^2}+ln\frac{(K-x_1)^2}{(K-x_2)^2}]\\
&+[\frac{1}{2}(k_1^2f_1+k_2^2f_2)-\frac{1}{2}(k_1^3+k_2^3)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(K+x_1)^2}{(K-x_1)^2}\\
&-[\frac{1}{2}(k_1^2f_1-k_2^2f_2)-\frac{1}{2}(k_1^3-k_2^3)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(K+x_2)^2}{(K-x_2)^2}\}.\qquad(28)\end{aligned}$$

Considering the case $K=x_{1,2}$ one can see that (28) still remains well defined. In the high energy limit we get again the simple formula:

$$\tilde{V}_{Sl}=-\frac{4e^2\pi}{K^2}\rho_1(\vec{r})\rho_2(\vec{r}-\vec{R})+O([\frac{k_i}{K}]^4)\qquad(29)$$

In the low-energy limit one obtains

$$\tilde{V}_{Sl}=-\frac{9\pi e^2\rho_1\rho_2}{k_1^3k_2^3}\{\frac{1}{2}k_1k_2(k_1^2+k_2^2)-\frac{1}{8}(k_1^2-k_2^2)^2ln\frac{(k_1+k_2)^2}{(k_1-k_2)^2}\}+O((\frac{K}{k_i})^2)\qquad(30)$$

and its $\hbar^2$ correction reads as:

$$\begin{aligned}\delta\tilde{V} &= -\frac{e^2}{9\pi^3}\{3k_1k_2(\frac{g_1}{k_1}+\frac{g_2}{k_2})-\frac{2k_1k_2}{(k_1^2-k_2^2)}(k_1f_1-k_2f_2)\\
&+\frac{1}{2}[(k_1f_1+k_2f_2)-\frac{3}{2}(k_1^2+k_2^2)(\frac{g_1}{k_1}+\frac{g_2}{k_2})]ln\frac{(k_1+k_2)^2}{(k_1-k_2)^2}\}+O([\frac{K}{k_i}]^2).\qquad(31)\end{aligned}$$

In the case $k_1=k_2$ one should take care about the correct consideration of the limit $k_1\to k_2$. In this case one should start from eq.(26) for the Yukawa force, put $k_1=k_2$ and make the limit

$\beta lim_{\beta\to 0}$. After path integration one will get at $k_1 = k_2$:

$$\delta\tilde{V} = -\frac{7e^2}{18\pi}[(\nabla k_1)^2 + (\nabla k_2)^2]. \tag{32}$$

It is very important to point out that the SL, CB or ETF approximations to the DM described in this section are used for calculating the exchange part of the DFM potential irrespective of the way that the density of each isolated nucleus is obtained. In the following we will refer to these potentials as SL, CB or ETF approaches to the DFM potential. Notice that for determining completely the DFM potential, the density of each isolated nucleus that enters through k_1 and k_2 in the previous formulas as well as the effective nucleon-nucleon force used have to be specified.

3 Results

In this Section we present the results for the DFM potential obtained using the different prescriptions considered in Section 2. The nuclear part of these potentials calculated with the realistic effective nucleon-nucleon force analyzed in this paper is attractive. Hence the relative momentum K in the local definition is always real when the energy exceeds the Coulomb barrier. On the other hand, the "frozen density" approximation, used in DFM, is still valid for fast enough collisions or, in other words, at rather high energies. The Coulomb barrier for the $^{16}O - ^{16}O$ system is about 10MeV. Therefore, we will consider only collisions above the Coulomb barrier where K is always real.

To check the validity of the ETF DM to the calculation of an ion-ion potential, we consider the exactly soluble HO model for the isolated nuclei. This model consists of describing the ground state of each colliding nucleus using HO wavefunctions. In this case the exchange part of the potential is easily calculated due to factorization of variables in the DM [11].

First of all, let us briefly describe the effective nucleon-nucleon force used in this paper. Here we will consider the Gogny force that is used in nuclear structure calculations and a MY3-type force that is typical in DFM calculations.

The effective Gogny force [10] consists of a finite-range Brink-Boeker term together with a density-dependent zero-range term

$$v(r) = \sum_{i=1}^{2}[w_i + b_i P^\sigma - h_i P^\tau - m_i P^\sigma P^\tau]exp(-\frac{r^2}{\mu_i^2}) + t_3(1 + x_3 P^\sigma)\rho^{1/3}(\frac{\boldsymbol{r}_1 + \boldsymbol{r}_2}{2})\delta(\boldsymbol{r}), \tag{33}$$

where P^σ and P^τ are the usual spin and isospin exchange operators, the coefficients w_i, b_i, h_i and m_i are the parameters of the central force and μ_i the range of the Gaussian form factor. The values of these parameters are given in [10]. In DFM calculations the density dependent term is taken in the so-called "sudden"approximation, which implies that the density of the composite system is simply the sum of individual densities: $\rho(\boldsymbol{r}) = \rho_1(\boldsymbol{r}) + \rho_2(\boldsymbol{r} - \boldsymbol{R})$ [13].

The density-dependent M3Y force is defined as

$$v(r) = F(\rho)g(E)v_{M3Y}(r), \tag{34}$$

where $v_{M3Y}(r)$ is the finite range of the M3Y Paris [15] or Reid-Elliott[14] force with a Yukawa-type formfactor. For a BDM3Y force the density-dependent term is given by [4]:

$$F_{BD}(\rho) = C(1 - \alpha\rho^\gamma), \tag{35}$$

while the DDM3Y force [17]reads:

$$F_{DD} = C(1 - \alpha e^{-\gamma\rho}). \tag{36}$$

Again, the density-dependent term is considered in the "sudden" approximation. The energy dependent term is taken as $g(E) = 1 - C_E E$.

In this paper we are going to consider the validity of different approximations to the DM for the calculation of the DFM potential rather than obtaining a realistic potential for describing the elastic scattering data. In order to do this wee will make the two following simplifications.

The first concerns the way that the ground state density of each isolated ^{16}O nucleus is calculated. To do this, we minimize the quantal ground state energy with respect to the oscillator parameter $\varepsilon = \sqrt{m\omega/\hbar}$. In the semiclassical calculations using the ETF, SL and CB approaches to the DM we first write the ground state energy using the Kohn-Sham [16] scheme (see reference [8] for more details) and then minimize with respect to the HO parameter. The binding energy and root mean square radius (RMSR) of the ^{16}O ground state obtained quantally and semiclassically (with the ETF, SL and CB approaches) are collected in Table 1. One can see that in all cases the results obtained with the ETF approach to the DM give a better description of the quantal ground state properties of ^{16}O than that obtained using the semiclassical SL or CB approximations to the DM. On the other hand, among the considered M3Y forces, the BDM3Y1*(Paris) force gives a RMSR that is very close to that obtained with the Gogny force

and consequently the same ground state density for the ^{16}O. Therefore, we will use the Gogny and BDM3Y1*(Paris) forces in our analysis.

The second remark deals with the definition of relative momentum K. If one uses the local definition of K and solves the system of equations: V=V(K); K=K(V) selfconsistently, the nuclear and Coulomb potentials are not separated. In this paper we are going to consider the different kinds of forces independently. For this reason and for the sake of simplicity we will use the global definition of K.

Now we consider the resulting $^{16}O -^{16} O$ ETF potentials calculated using the quantal HO density for each ^{16}O nucleus and the Gogny and BDM3Y1* forces. In Figure 1 these potentials calculated at several energies are displayed by dashed and solid lines respectively. The upper dashed line is the energy independent sum of the Brink-Boeker and zero-range direct parts of the DFM potential in the Gogny force case. Thus, the difference between the full potential and this energy independent direct part gives the contribution of the one-particle exchange due to the finite (energy dependent) and zero (energy independent) ranges of the Gogny force. One can see that at low energies the total potential is purely attractive due to the exchange interaction coming from the finite-range part of the Gogny force. When the energy increases, the total DF potential tends to its energy independent part (direct Brink-Boeker and full zero-range contributions). This latter potential is repulsive at small distances and attractive when the separation between the nuclei is increased and tends to zero at large distances.

As can be seen from eq.(34), the BDM3Y1 force depends linearly on the energy. This force has two essential differences when compared with the Gogny interaction. First of all, in this case the direct DFM potential (3) is energy dependent. The upper solid line corresponds to this direct potential in the $E = 0$ case. On the other hand, taking into account the linear energy dependence of the BDM3Y force and the inverse energy dependence of the exchange potential (22) (in the high-energy limit) one sees that the exchange potential in this case does not vanish when the energy tends to infinity and, consequently, the total potential does not tend to the direct part in this limit. The total and direct ETF DFM potentials obtained with the BDM3Y1* force are also displayed in Figure 1. Looking at this figure one can see that in the region of energies of physical interest ($E_{cm} < 1000MeV$) the total DFM potentials obtained using quantal HO densities and Gogny and BDM3Y1* forces are very similar. At higher energies they start

to show differences. However, these differences should be considered only in the mathematical aspect because the nucleus-nucleus potentials at these high energies can not be defined correctly.

Now we turn to the discussion of the validity of different approximations to the DM for calculating DFM potentials considered in the present paper. As was pointed out above, the exchange effects are larger at small energies and their contribution falls when the energy increases. Therefore it is reasonable to expect that the influence of the different approaches to DM on the DFM potential will be more important at low energies. Hence to investigate the applicability of the different approximations to the DM for calculating the DFM potential, we will consider the static case (K=0). To this aim we define a function σ(D), which is the deviation of the approximate total DFM potential with respect to the exact potential:

$$\sigma(D) = \frac{V_{SL,CB,ETF}(D) - V_{exact}(D)}{V_{exact}(D)}, \tag{37}$$

where $V_{exact}(D)$ is the DFM potential calculated with the quantal HO DM at a separation distance D, whereas V_{SL}, V_{CB} or V_{ETF} are the DFM potentials calculated with the SL, CB or ETF approximations. We perform two sets of calculation using two different densities for the isolated ^{16}O nucleus to obtain the V_{SL},V_{CB} and V_{ETF} for the Gogny and BDM3Y1*forces.

In the first case we used the densities that minimize the ground state Kohn-Sham energy calculated in the SL, CB or ETF approach for an uncharged ^{16}O nucleus. In other words this case corresponds to the selfconsistent calculation, where the same approach to the DM is used to obtain the DFM potential and the density of each isolated nucleus.

These results are plotted in Figures 2 and 3 for the Gogny and BDM3Y1* forces respectively. These figures clearly show that the DFM potential V_{ETF} calculated using the selfconsistent ETF densities reproduces better the quantal DFM potential than V_{SL} or V_{CB} calculated with the selfconsistent SL or CB densities. This result is obvious if one takes into account that for an isolated ^{16}O nucleus the selfconsistent density in the ETF approximation is closer to the quantal density as compared with the other approximation to the DM, as can be seen from Table 1.

In the second set we obtain the different DFM potentials using the quantal HO density for each ^{16}O nucleus and the Gogny and BDM3Y1* forces. The results for the function σ(D) are plotted in Figures 4 , 5 and 6 for the Gogny, BDM3Y1* and Coulomb forces respectively.

In this case the situation is more complicated. From Figures 4 and 5 one can see that V_{SL}

(dotted line) does not reproduce the quantal potential for distances $D > 3$fm. The potential V_{ETF} (dashed-dotted line) is very close to the quantal DFM potential for $D < 6$fm. If $D > 6$fm, V_{CB} (dashed line) gives the best agreement with the quantal DFM potential, while for $D < 6$fm it works slightly worse than V_{ETF}. At large distances $R \approx 10$ fm, the nuclear part of the nucleus-nucleus potential is very small wh compared with its Coulomb part. Consequently, the rather strong deviation (within 10%) shown by the the nuclear part is not very important. However, from the formal point of view one should take it into account.

As is discussed in [8] all the considered approximations to the DM (SL, ETF or CB) are actually distributions. They are very efficient for obtaining expectation values, but there is no reason for reproducing the quantal DM at each point in coordinate space. If one looks for the asymptotic behaviour of the different approximations to the DM considered in this paper, one can see that at finite s, the SL and CB DM behave as : $\rho(R,s) \propto 2C\alpha^2R^2\exp[-\alpha^2R^2]$ when $R \to \infty$ (more precisely when $\alpha R >> 1, R >> s$), where C is the normalization constant. The ETF DM has a different asymptotic behaviour: $\rho(R,s) \propto 2C\alpha^2R^2(1-\frac{2}{27}\alpha^4s^2R^2)exp[-\alpha^2R^2]$. At the same time the quantal DM asymptotically behaves as $\rho(R,s) \propto 2C\alpha^2R^2exp[-\alpha^2R^2]$. One can see that at very small s and large R the SL, CB and ETF DM are similar to the quantal density matrix. However, when s is increased, the ETF DM starts to deviate from the quantal values. Due to the extra R^2 dependence, the ETF DM gives a worse approximation to the quantal DM as compared with SL and CB DM if one uses the same quantal HO density for obtaining the different approaches to the quantal DM.

This lack of accuracy of the ETF DM in describin the quantal DM is not important when one calculates the ground state properties of isolated nuclei. In the region of wrong asymptotic behaviou the DM is too small to give any significant contribution to the total energy as can be seen from Table 1. However, for calculating DFM potentials the situation is different. The values of densities over all the nucleus contribute to the DFM potential at large distances Therefore,the wrong asymptotic part of the ETF DM can give a significant contribution to the DFM potential at large separaon distances. Thus, we come to the conclusion that the DFM potential is a more sensitive tool for investigating the one-particle density matrix in nuclei than fully integrated quantities such as the binding energy or RMSR.

For improving V_{ETF} calculated with the quantal HO density at large separation distances

D, we can make the following modification of the ETF DM. We introduce a cutoof radius R_{co} that removes the h^2 correction from the SL DM. Therefore this new ETFM DM is is just the ETF DM when $R < R_{co}$ and the SL DM if $R > R_{co}$ and has the right asymptotic behaviour for large R values. The results of the DFM potential calculated with this new ETFM DM are displayed in Figures 4, 5 and 6 by solid lines. It is clear that this new approximation gives a better description of the exact DFM potential at all distances D. However, a new parameter, the cutoof radius in the outer region, is introduced in this case. The solid line corresponds to the approximated DFM potential obtained with this modified ETF DM (V_{ETFM}), where the $\hbar^2$ contribution has been cut off after R_{co}. One can see that V_{ETFM} agrees to within 1% with the quantal DFM potential.

In Figure 6 we show the results for the long-range Coulomb force. For $D < 4$fm V_{SL} gives a better result than V_{CB} and at $D > 4$fm it starts to deviate from the t quantal DFM potential values. The V_{ETF} gives a very good description of the quantal DFM potential and gives an error within 0.25% if $6 < D < 12$fm. Furthermore, for the Coulomb case the use of V_{ETFM} significantly improves the agreement with the quantal DFM potential in all of the considered region.

It is also interesting to consider in our model calculations the height and position of the Coulomb barrier. The results corresponding to the selfconsistent calculations are collected in Table 2. In this case the ETF DFM potential gives a clearly better approximation to the exact quantal values when compared with SL and CB DFM approaches. This result is obvious if one takes into accountthe fact that the selfconsistent density for the ETF case is very close to the quantal density. The height and position of the Coulomb barrier calculated with the different approximations to the DFM potential obtained with the same quantal density are shown in Table 3. In this case one can see that the better agreement with the quantal results is obtained using the CB approach to the DFM potential. To improve the ETF DM potential we again use the ETFM approxiationto the DM where a cutoof radius R_{co} is introduced. First of all,from Fig.4-6 one can obtain the following conclusion: the longer the range of the force, the smaller the value of cutoof radius that should be used to reproduce the quantal DFM. The Coulomb barrier comes from the superposition of longe-range Coulomb force ($R_{co} = 5fm$) and a shorter-range nuclear force. We choose the cutoof radius $R_{co} = 5.5fm$ and $R_{co} = 5fm$ for the Gogny and

BDM3Y1* forces respectively. One can see that the ETFM DFM potential nicely reproduces the quantal result for both forces. From Table 3 one can also see thatthe the Gogny and BDM3Y1* interactions give very close results for the Coulomb barriers.

4 Summary

In this paper we have derived the one-particle exchange contribution to the DFM potential using the recently proposed ETF approach to the DM. We consider here nucleon-nucleon forces with the widely used Gauss, Yukawa and Coulomb form factors. As representative examples of these forces, we have performed our numerical analysis with the Gogny and BDM3Y1* effective interactions.

To obtain the densities of each isolated ^{16}O nucleus, we have used trial HO wavefunctions. The oscillator parameter $\varepsilon = \sqrt{m\omega/\hbar}$ is obtained by minimizing the exact ground state energy in the quantal case and the corresponding Kohn-Sham energy when the quantal DM is replaced by its SL, CB or ETF approximations.

If each self-consistent density (SL, CB or ETF) is used for obtaining its corresponding DFM potential, it is found that the ETF potential gives a better description of the quantal one than the SL and CB DFM potentials.

However, if one uses the same selfconsistent quantal density to obtain all the approximated DFM potentials, the situation is more complicated. First of all,it is clearly seen that the SL approach to the DFM potential compares worse with the quantal potential than the CB or ETF approaches. In all the analyzed cases the ETF approach to the DFM potential gives a better description of the quantal potential at small and intermediate separation distances ($D < 6fm$) when compared with the potential obtained in the CB approximation. However, at large separation distances, the ETF approach fails in describing the quantal potential. From a physical point of view, this is not very important because the nuclear part of the total ion-ion potential is very small at these distances. The reason for this deviation of the ETF potential from the quantal potential is due to the different asymptotic behaviour of the quantal and ETF DM of each isolated nucleus. To improve the ETF DM of each nucleus at large distances, we drop its $\hbar^2$-contribution after a cutoof radius R_{co}. In this way one obtains a modified DM which

coincides with the full ETF DM at $R < R_{co}$ and with its SL part DM if $R > R_{co}$. We have numerically shown that this ETFM DM produces a DFM potential in very good agreement with the quantal result in the whole range of distances.

Hence we reach the conclusion that the DFM potential is a sensitive tool for investigating the quality of the approximations to the DM in the whole range of R-values. While in the calculations of ground state properties of nuclei the asymptotic behaviour of the DM is suppressed by the small values of the particle density at large R, in the calculation of the DFM potentials it is clearly revealed.

5 Acknowledgments

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6 Table Captions

Table 1. Binding energy and root mean square radius $< r^2 >^{1/2}$ of an uncharged ^{16}O nucleus calculated with trial HO wavefunctions quantally (QM) and using the SL, CB and ETF approximations to the density matrix. The results obtained with the Gogny and several M3Y forces are displayed. The centre-of-mass correction to the energy has been taken into account. The HO parameter which minimizes the binding energy for each force is given by $\alpha = 3/2 < r^2 >^{-1/2}$.

Table 2. Height (V_B) and position (R_B) of the Coulomb barrier calculated with the quantal DFM potential (QM) and with its SL, CB and ETF approximations using the corresponding selfconsistent densities for the Gogny and BDM3Y1* forces.

Table 3. The same as Table 2 but with the SL, CB and ETF DFM potentials obtained with the quantal density.

Figure 1. Direct and exchange contributions at several energies to the ETF DFM potential calculated with the quantal density. Solid and dashed lines correspond to the results obtained with the BDM3Y1* and Gogny forces respectively.

Figure 2. Relative deviation from the quantal DFM potential with respect to its SL (dotted), CB (dashed) and ETF (solid) approximations obtained with the corresponding selfconsistent density and the Gogny force.

Figure 3. The same as Figure 2, but for the BDM3Y1* force.

Figure 4. Relative deviation from the quantal DFM potential with respect to its SL (dotted), CB (dashed), ETF (dashed-dotted) and ETFM (solid) approximations using the quantal density and the Gogny force.

Figure 5. The same as Figure 4, but for the BDM3Y1* force.

Figure 6. The same as Figure 4, but for the Coulomb force.

Table 1

	E_{QM}	$< r^2 >^{1/2}_{QM}$	E_{SL}	$< r^2 >^{1/2}_{SL}$	E_{CB}	$< r^2 >^{1/2}_{CB}$	E_{ETF}	$< r^2 >^{1/2}_{ETF}$
Gogny	-138.07	2.63	-129.49	2.67	-133.80	2.65	-134.35	2.66
BDM3Y1	-121.15	2.55	-112.67	2.57	-114.63	2.57	-115.76	2.56
BDM3Y2	-114.57	2.53	-105.54	2.55	-107.82	2.54	-109.21	2.53
BDM3Y3	-110.69	2.52	-101.46	2.53	-103.86	2.53	-105.33	2.52
BDM3Y1*	-115.57	2.63	-107.94	2.65	-109.70	2.65	-110.44	2.63
DDM3Y*	-122.29	2.67	-115.17	2.70	-116.69	2.70	-117.13	2.68

Table 2

	QM	SL	CB	ETF
		Gogny		
$R_B(fm)$	8.36	8.51	8.42	8.38
$V_B(MeV)$	10.35	10.18	10.27	10.35
		BDM3Y1*		
R_B	8.46	8.57	8.50	8.43
V_B	10.18	10.06	10.12	10.24

Table 2

	QM	SL	CB	ETF	ETFM(R_{co}=5fm)
			Gogny		
$R_B(fm)$	8.36	8.40	8.35	8.35	8.37
$V_B(MeV)$	10.35	10.31	10.36	10.38	10.35
			BDM3Y1*		
$R_B(fm)$	8.46	8.51	8.45	8.40	8.45
$V_B(MeV)$	10.18	10.13	10.19	10.25	10.19

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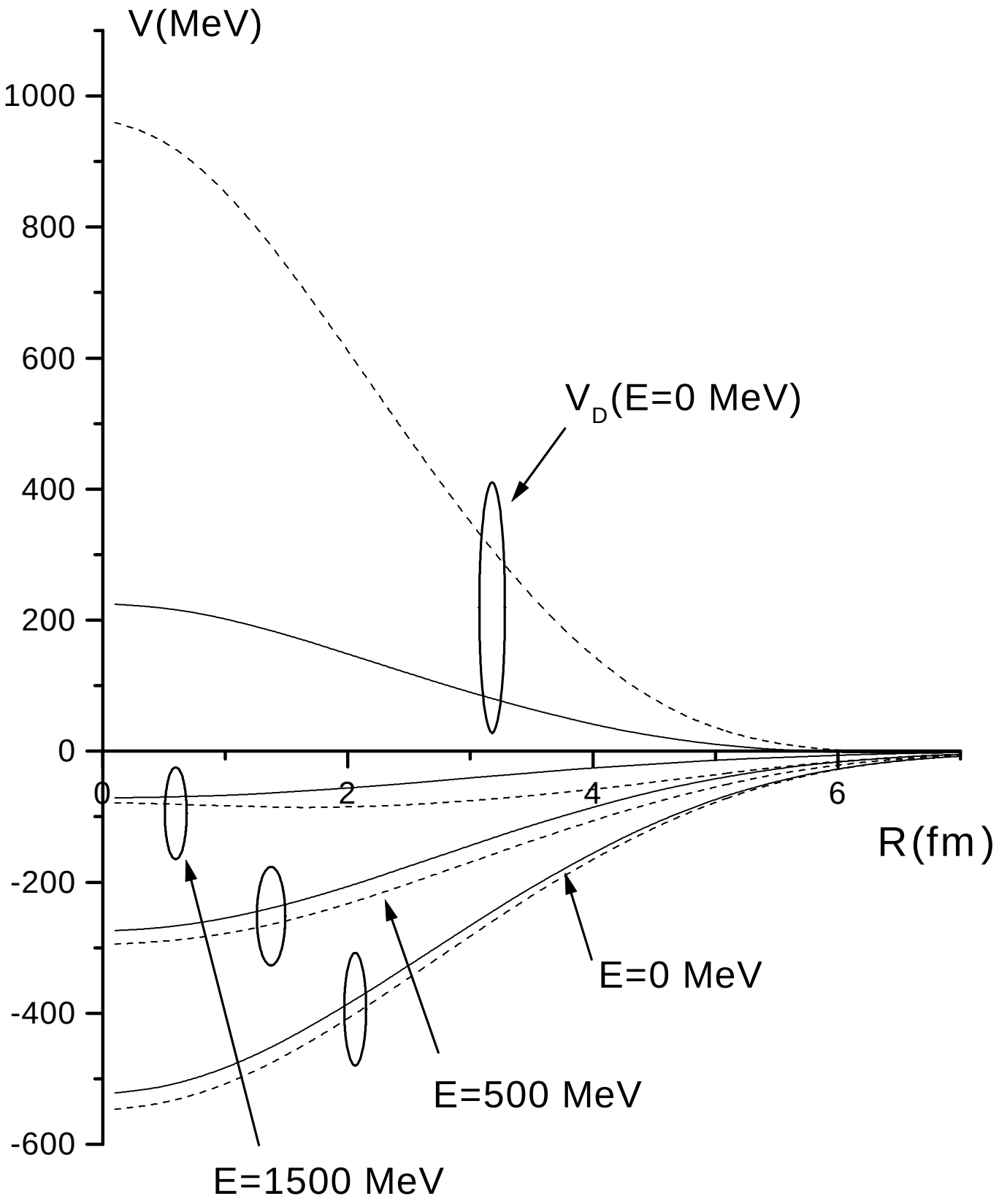
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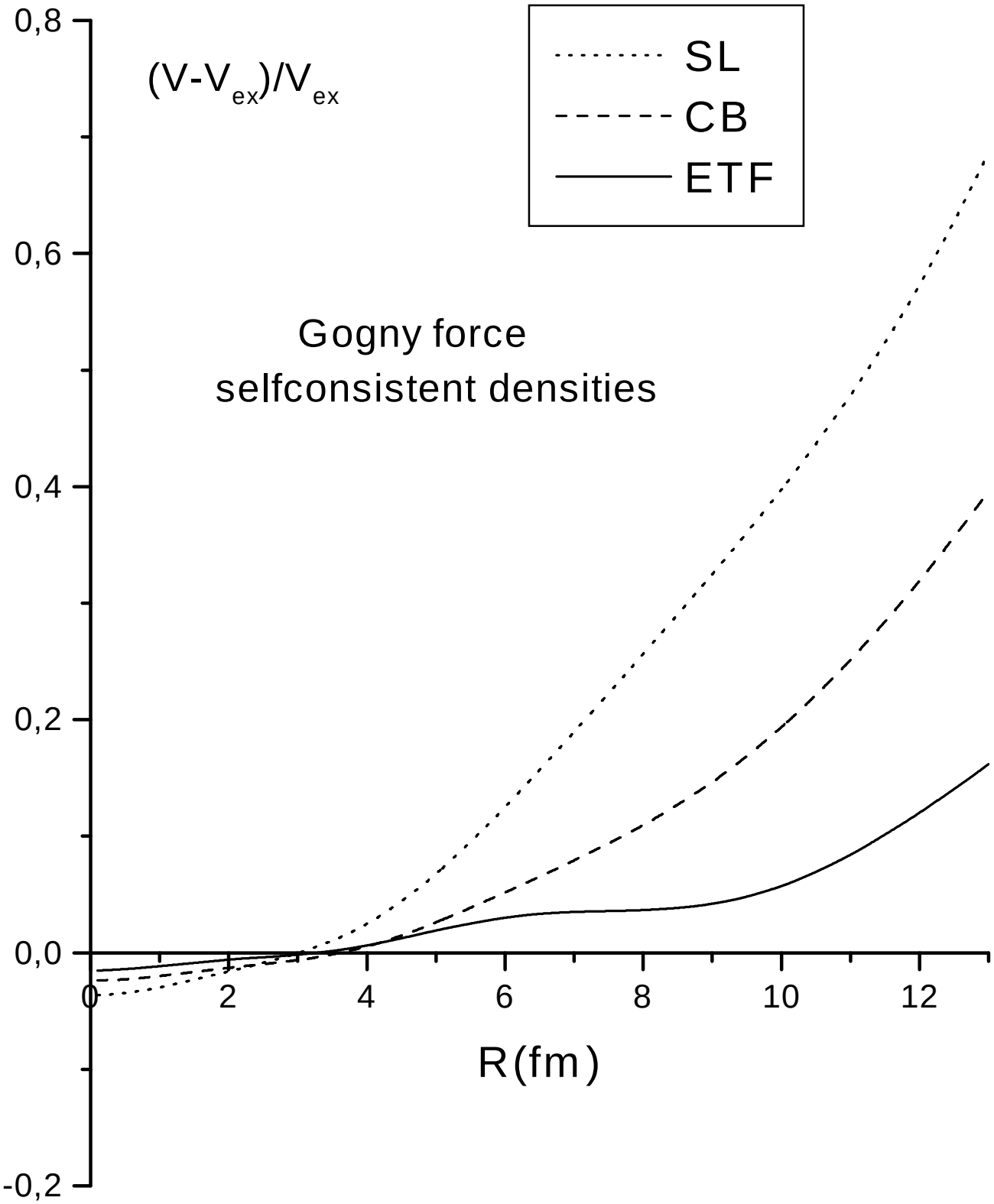
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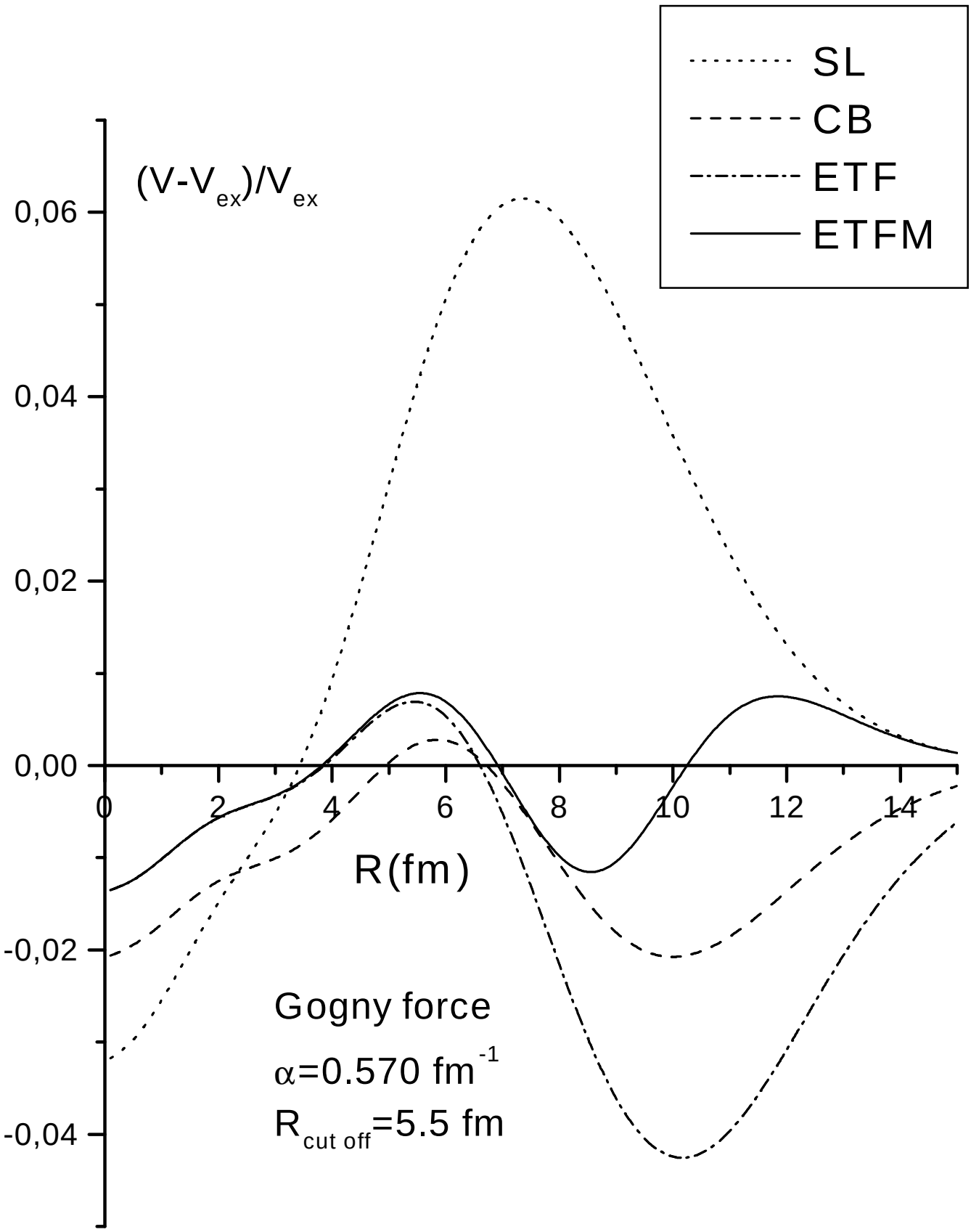
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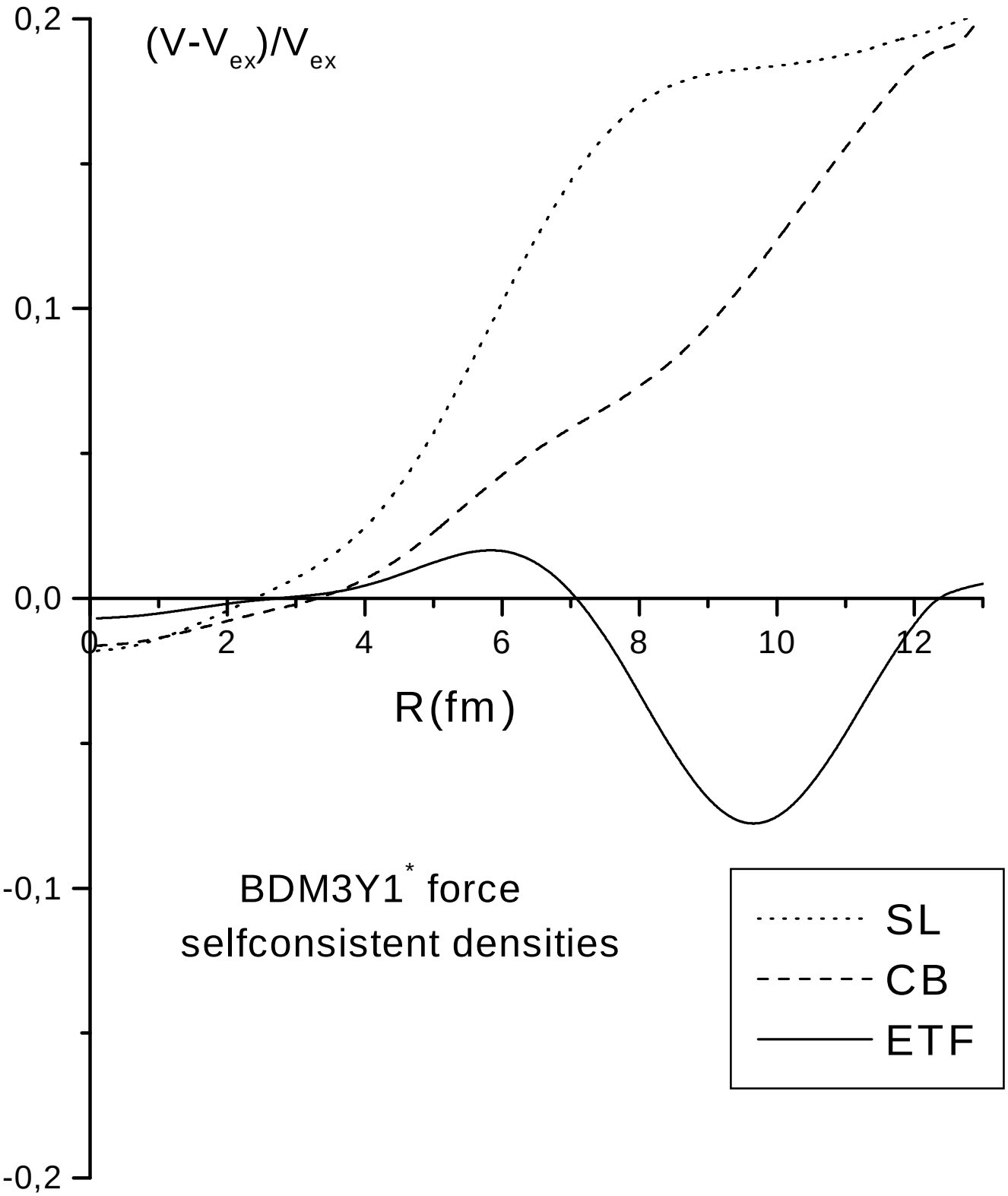
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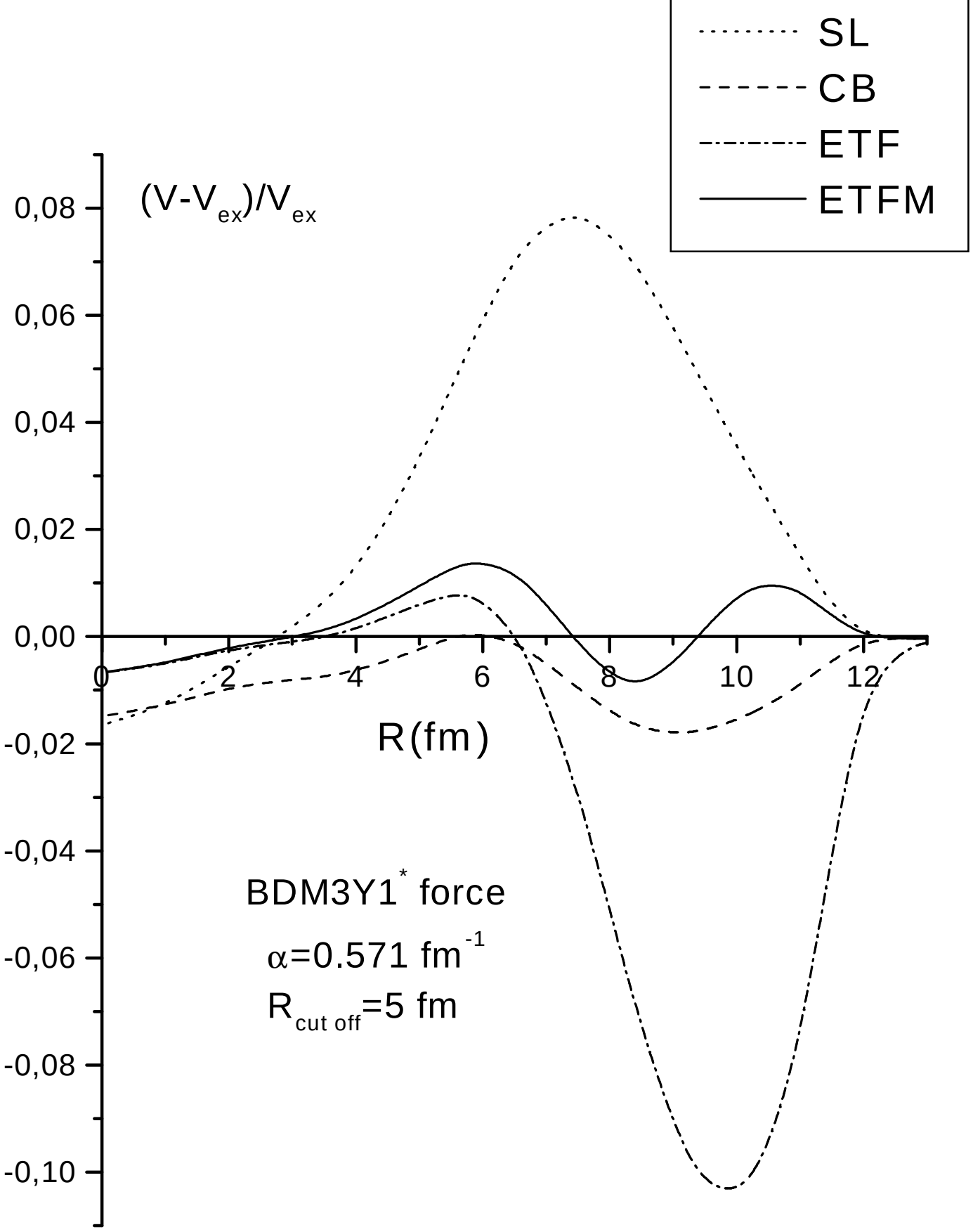
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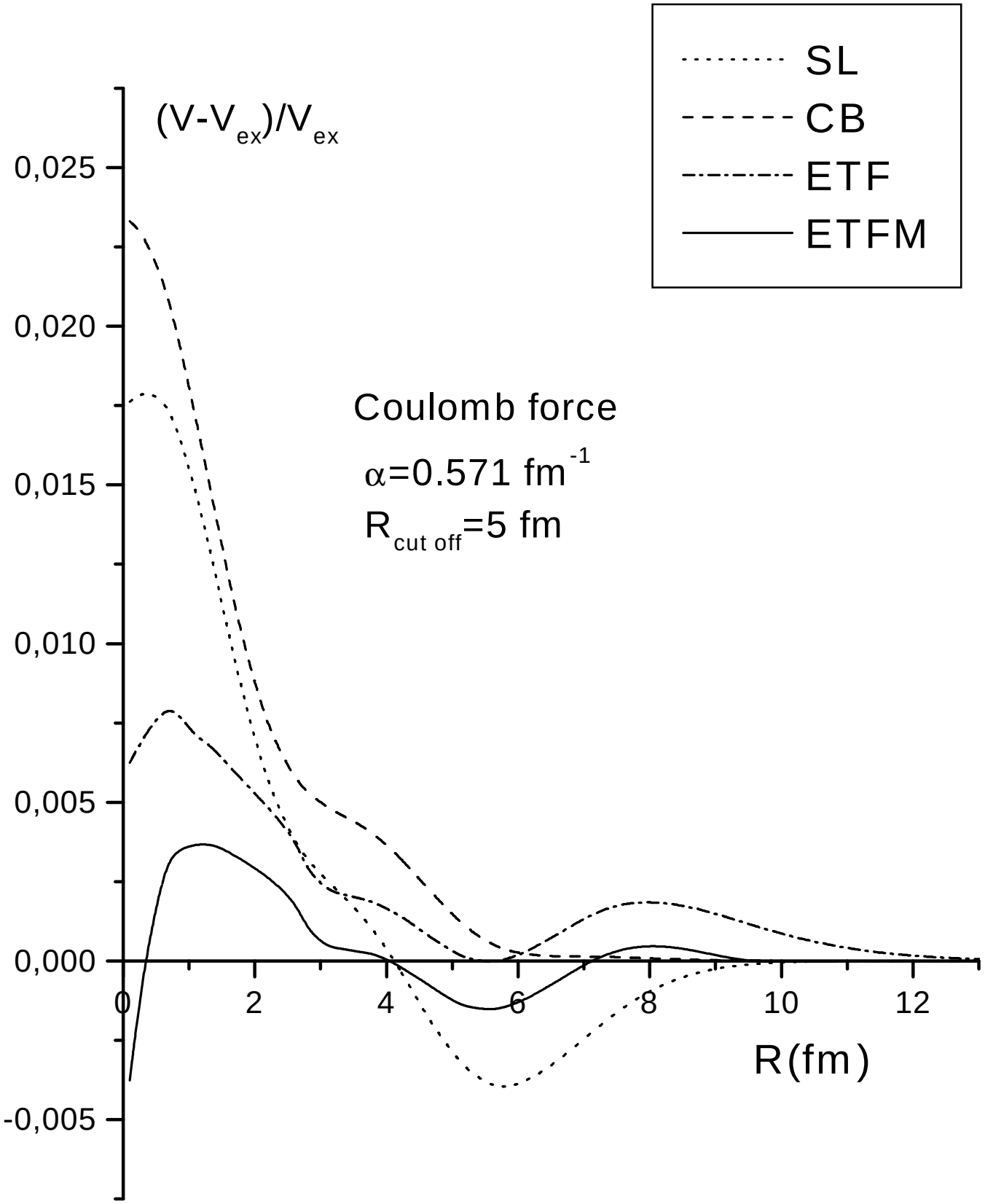
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